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The electronic structure and magnetism of the Al/Fe interfaces

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Abstract

The electronic structure and magnetic properties of the Fe(001) surface with Al overlayers, vice versa, are studied by means of ab initio band structure calculations using the LSW method. An Fe–Al(001) multilayer system is calculated for comparison. The calculations show that Al reduces the magnetic moments of the interface iron. The Al interface layer has a small negative magnetic moment. The interaction between the interface Al and Fe layers, and the intra-atomic exchange splitting are discussed.

Keywords: A. Interfaces; A. Multilayers; A. Metals; C. Ab initio calculations; D. Magnetic properties

1. Introduction

The electronic structure and magnetic properties of the iron (001) surface and interfaces have been studied quite extensively [1–4]. Band structure calculations for the clean Fe(001) surface showed surface states with a strongly enhanced magnetic moment [1–3,5,6], in contrast with the early experimental results [7,8]. As a function of depth the layered-resolved magnetic moments and charge show an oscillatory behavior for the clean Fe(001) surface [5,6,9–11]. When an Fe(001) surface is covered by a layer of the noble metals (Ag or Au) the oscillations of the charge and magnetic moments disappear. The interface Fe has a magnetic moment of about $2.6\mu_B$, some between the clean surface and the bulk values, and the interface noble metal atom has a small positive magnetic moment (about $0.1\mu_B$) [11,12]. Wu and Freeman calculated the Fe(001) surface covered by a monolayer of Mn. They found large magnetic moments (about $3.2\mu_B$) for the Mn atoms with an anti-ferromagnetic structure, and reduced magnetic moments for the interface iron [13]. The interface Fe covered by a monolayer or bilayer of the early 3d transition metals (Ti, V or Cr) has a reduced magnetic moment, while the interface Fe covered by the late 3d transition metals (Co or Ni) has an enhanced moment, as compared with the bulk value [9,10,14,15].

A free Fe(001) monolayer has a large magnetic moment (about $3.2\mu_B$). Fu et al. showed that the Fe(001) monolayer on a noble metal surface or sandwiched by noble metals has a magnetic moment of about $2.9\mu_B$ [16,17]. However, the band structure calculations [18,19] for a sub-monolayer of iron on the W(001) surface show a magnetically 'dead' layer when the Fe films are thinner than or equal to one monolayer if only a ferromagnetic solution is considered.

Aluminum is generally regarded as a metal with almost-free valence electrons and does not possess any d-electrons. Interestingly, Fuss et al. [20] found that the Al–Fe multilayer system shows an anti-ferromagnetic coupling. Recently Schulze et al. [21], using the very surface-sensitive low-energy ion scattering spectroscopy (LEISS), found that at room temperature (25°C) at high dose rates, the Al grows on the Fe(001) surface in a layer-by-layer mode, forming largely bulk-like aluminum overlayers which do not react readily to form an alloy.

Isshiki et al. determined the electronic structure of a bilayer of Fe on the Al(001) surface, using the self-consistent charge discrete variational X_α method [22]. They found that the magnetic moment of the interface Fe layer is $3.3\mu_B$, which is substantially enhanced as compared with the bulk value $2.15\mu_B$ found by the same authors [22]. However, it was found by Perez-Diaz and Munoz using an empirical tight-binding method for an Fe–Al multilayer that the magnetic moment of the interface iron has been reduced by as much as 24% [23]. The results of Isshiki et al. [22] were also in contrast to the reduction of the magnetic moment for the analogous Ni/Al system [24].

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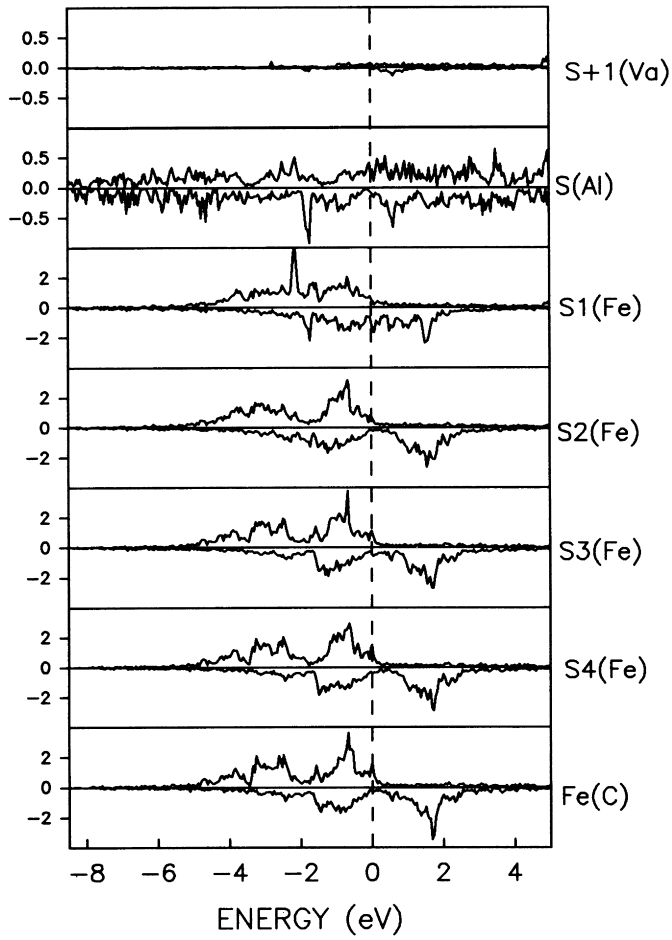

Fig. 1. Layer-resolved DOS of the A1/Fe (001) system. The positive values represent for the majority electrons and the negative values for minority electrons. The Fermi level is at the zero energy, the same for the following figures.

In this paper we present a systematic study of the Al–Fe interface by means of ab initio band structure calculations with the Localized Spherical Wave (LSW) method and the slab (super-cell) approach. The calculations were performed for the Fe(001) surface covered by a monolayer of Al, a monolayer or bilayer of Fe on the Al(001) surface, and a monolayer of Fe inserted into Al, as well as an Fe–Al multilayer system. The structures are assumed ideal without interdiffusion. The interface interactions and their influence to the interface magnetic properties are discussed.

2. Details of calculations

Ab initio band structure calculations were performed with the Localized Spherical Wave (LSW) method [25] using a scalar-relativistic Hamiltonian. We used the spinpolarized local-density exchange-correlation potentials [26] inside space-filling, and therefore overlapping spheres around the atomic constituents. The self-consistent calculations were carried out including all core electrons. We performed iterations for the large systems with 375 or 648 k-points disturbed uniformly in an irreducible part of the Brillouin zone (BZ), corresponding to a volume of the BZ per k-point of the order of 1×10^{-6} Å^{-3}. Self-consistency was assumed when the changes in the local partial charges in each atomic-sphere decreased to the order of 1×10^{-5}.

In the construction of the LSW basis [27,28], the spherical waves were augmented by solutions of the scalar-relativistic radial equations indicated by the atomic symbols 4s, 4p, and 3d; and 3s, 3p and 3d for Fe and Al, respectively. The internal 1 summation used to augment a Hankel function at surrounding atoms, was extended to $l = 3$, resulting in the use of 4f orbitals for Fe and Al. For the surface systems the vacuum is occupied by empty spheres (Va), for which the functions 1s and 2p, and 3d as an extension, were used. The Wigner–Seitz spheres of the Fe and Al atoms are the same as the corresponding bulk values.

Table 1
Calculated results of the Al/Fe(001) system (magnetic moment (M) and valence electrons (electrons) in the atomic sphere from the surface (S) to the center)

Layer	M (μ_B)	Electrons
C(Fe)	2.27	8.00
S − 4(Fe)	2.27	8.00
S − 3(Fe)	2.27	8.00
S − 2(Fe)	2.34	7.99
S − 1(Fe)	2.33	8.03
S(Fe)	1.69	8.01
S + 1(Al)	−0.06	2.74
S + 2(Va)	0.01	0.21

The systems calculated were as following: The Fe(001) covered by a monolayer of Al is composed of 11 layers of iron with on each side one monolayer of Al (Al/Fe system, in short). The systems of the Al(001) surface covered by iron are composed of seven layers of Al with on each side a bilayer of iron (Fe_2/Al) or a monolayer of Fe(Fe_1/Al). The Al–Fe multilayer system is consisted of eleven layers of Fe and seven layers of Al. Also one Fe(001) monolayer is inserted in nine layers of Al (Al/Fe/Al). Experimentally it was observed that iron grows on Al(001) with a 45° rotation [29]. In our calculations we take a tetragonal unit cell with a- and b-axis the same as a-axis of the fcc Al, and the iron with 45° rotation to the bcc iron lattice (Fe(110)/Al(001)). The lattice match between the two metals (a of fcc Al compared with $a\sqrt{2}$ of the bcc Fe) is very good (mismatch is about 0.1%). The interlayer distance (1.73 Å) between the interface iron and aluminum is the average distance of the interlayer Al–Al layers (2.03 Å) and Fe–Fe layers (1.43 Å). And the Fe–Al distance for the interface layers is 2.67 Å, about the average value of the bulk Al–Al and Fe–Fe distances. It is noted that our structure arrangement for the Fe_2/Al structure is different from the corresponding structure by Isshiki et al. [22]. In their calculations the a-axis of the iron layers was expanded by $\sqrt{2}$, as shown in Fig. 1 of Ref. [22]. The vacuum distances between the slabs are large (>10 Å) to avoid the inter-slab interaction in our calculations.

3. Results of the calculations

3.1. Fe(001) surface covered by a monolayer of Al

The calculated results (magnetic moments and valence electrons of iron in the Wigner–Seitz spheres) are listed in Table 1. Fig. 1 shows the layer-resolved densities of states (DOS).

The interface iron is almost neutral (8.01 electrons). The surface aluminum loses about 0.26 electrons, most of which is spill-over to the vacuum. The interface iron has a strongly reduced magnetic moment of 1.69μ_B, as compared with the bulk value 2.26μ_B found in our former work [11], which is in contrast to the enhanced moments for the clean Fe(001)

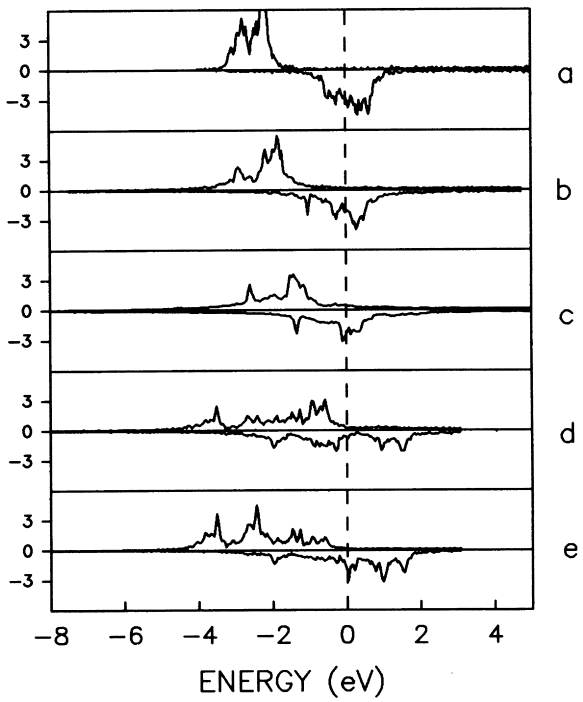

Fig. 2. DOS of the surface (or interface) Fe layer for the free Fe(001) monolayer: (a) Fe_1/Al; (b) Al/Fe/Al; and (c) Fe_2/Al(001). ((d) For the surface Fe layer and (e) for the interface Fe layer.)

Table 2
Magnetic moment and valence electrons in the atomic sphere of iron for the Fe_2/Al, Fe_1/Al, Al/Fe/Al systems as compared with the free Fe(001) monolayer (Fe ML) and the clean Fe(001) surface. For Fe_2/Al(001) system, S represents for the surface Fe atom, and S − 1 represents for the interface Fe layer

	M (μ_B)	Electrons
Free Fe ML	3.10	7.16
Fe(001) surface	2.91	7.50
Fe(bulk)	2.26	8.00
Fe_2/Al(001)	2.90(S)	7.52
	1.71(S − 1)	8.10
Fe_1/Al(001)	2.48	7.45
Al/Fe/Al	1.65	7.97

surface (about $2.91\mu_B$) [11,12], and the Au/Fe(001) ($2.55\mu_B$) [11], and the Ag/Fe(001) ($2.52\mu_B$) [12]. The convergence of the magnetic moments as a function of depth from the surface is not smooth. The magnetic moment of Fe layers increases from $1.69\mu_B$ for the interface layer to $2.33\mu_B$ for the next layer, and to $2.34\mu_B$ for the third iron layer. From the forth layer it converges to the bulk value. The reduction of the interface Fe magnetic moment is due to the increased occupation of the minority 3d orbitals (2.47 electrons) and the decreased occupation of the majority 3d orbitals (4.20 electrons), as compared to the bulk values (2.10 and 4.42 electrons, respectively). The surface Al has a small negative magnetic moment.

The calculations for the Fe(001) surface covered by a monolayer of Al with a larger Al–Fe distance (2.867 Å, the Al–Al distance in the metal) show sensitivity to the distance. The difference mainly exists for the interface layer: the interface Fe has a larger moment ($1.92\mu_B$).

Fig. 1 shows layer-resolved densities of states for the Al/Fe(001) system. The density of states for iron bulk and for a clean iron (001) layer is included in Fig. 2, for comparison. The interface iron in the Fe/Fe(001) system has four nearest iron neighbors and four nearest aluminum neighbors, which is different from the bulk iron (eight nearest iron neighbors) and from the clean Fe(001) iron (four nearest iron neighbors) [11,12]. The crystal field splitting for the interface Fe 3d states is not very clear, as shown in Fig.1. However, the widths of the Fe 3d bands are the same as the bulk values, and the partial density of sates of the 3d bands is more similar to that of the bulk than to that of the clean Fe(001) surface. The band of the minority electrons is filled more as compared with the bulk, which is consistent with the electronic configurations as shown in Table 1.

3.2. The Al(001) surface covered with iron

Table 2 shows that the calculated magnetic moments and valence electrons of iron in the Wigner–Seitz spheres for the Al(001) surface covered by a bilayer of Fe (the Fe_2/Al(001) system). The surface Fe has a magnetic moment of $2.90\mu_B$ and 7.52 electrons, which is comparable to the clean Fe(001) surface ($2.91\mu_B$, and 7.50 electrons, respectively [11]). The interface Fe has a reduced magnetic moment of $1.71\mu_B$, as compared with the bulk value. This result is in contrast to that proposed by Isshiki et al., who found that for the Fe_2/Al(001) system the interface Fe has an enhanced magnetic moment ($3.3\mu_B$).

Table 2 also includes the magnetic moments of the Fe atoms for the free Fe(001) monolayer, Fe_1/Al(001) and Al/Fe/Al systems.

The free Fe(001) monolayer shows a strong spin-polarization (magnetic moment $3.10\mu_B$), which is reduced to $2.48\mu_B$ when put onto the Al(001) surface. Furthermore the magnetic moment of the Fe in the Al/Fe/Al system is reduced strongly to $1.65\mu_B$. The neighboring aluminum atom has a small anti-ferromagnetic moment ($-0.05\mu_B$).

To provide a better understanding of the mechanism behind the strong reduction of the magnetic moments for the Fe sites, we show in Fig. 2 the densities of states within the atomic spheres of the Fe layers for the free Fe(001) monolayer, Al/Fe/Al, Fe_1/Al(001) and Fe_2/Al(001) systems.

The free Fe(001) monolayer has the band structure reflecting the reduced coordination: narrow 3d bands (about 2 eV). The wide Fe 4s, 4p bands and the larger splitting in the 3d bands for both majority and minority electrons are due to the interaction with the 4 neighboring iron atoms with a distance of 2.867 Å. The 3d bands for the majority electrons are about 2 eV below the Fermi energy, and are almost fully occupied. The minority 3d bands are near the Fermi level (from about −0.9 to 1.2 eV). Such results are consistent with the large difference in the occupation of the Fe 3d orbitals: 4.76 electrons for the majority 3d states, and 1.71 electrons for the minority 3d orbitals. The exchange splitting is large (2.75 eV). The shapes of the densities of states for the Fe 3d states for the free Fe(001) monolayer, Fe_1/Al(001) and Al/Fe/Al systems are similar. However, there are some systematically changes: the band widths of the 3d states increase with increasing the number of the Al neighbours (about 2.0, 2.4 and 2.6 eV for the free Fe(001) monolayer, Fe_1/Al(001) and Al/Fe/Al, respectively). The center of the 3d bands for the majority electrons shifts up closer to the Fermi level with the increasing number of the aluminum neighbors, which is consistent with the decreasing of the magnetic moments as shown in Table 2. The densities of states at Fermi level for all the three cases for the minority electrons are higher than the bulk value, as shown in Figs. 1 and 2.

The 3d bandwidths for the Fe_2/Al(001) system are much broader than that of the monolayer of Fe supported by Al(Fe_1/Al), due to the strong Fe–Fe interactions. The band structure of the surface Fe layer in the Fe_2/Al(001) system is comparable to that of the clean Fe(001) (Fig. 2), expect some small difference in the structure due to the difference of the number of the next-nearest neighboring Fe atoms. The Al substrate has little influence on the surface Fe layer.

Table 3
Calculated results of the Al–Fe multilayer system: magnetic moment (M) and valence electrons (in the Fe 4s, 4p 3d and 4f, and Al 3s, 3p 3d and 4f states) in the atomic sphere in each layer from the interface (S) to the center

	M (μ_B)	Electrons				
		s	p	d	f	Total
C(Fe)	2.25	0.64	0.77	6.53	0.06	8.00
S − 4(Fe)	2.27	0.64	0.77	6.53	0.06	8.00
S − 3(Fe)	2.27	0.64	0.77	6.53	0.06	8.00
S − 2(Fe)	2.32	0.64	0.77	6.53	0.06	8.00
S − 1(Fe)	2.28	0.65	0.77	6.55	0.06	8.02
S(Fe)	1.89	0.59	0.69	6.61	0.04	7.94
S(Al)	−0.09	1.09	1.51	0.41	0.06	3.07
S − 1(Al)	−0.01	1.14	1.40	0.38	0.03	2.96
S − 2(Al)	−0.01	1.15	1.42	0.40	0.04	3.01
C(Al)	0.00	1.14	1.44	0.38	0.04	3.00

3.3. The Al–Fe multilayer system

To obtain a better understanding of the interactions between the interface Al and Fe, we performed band structure calculations for a multilayer structure. The calculations show that there is a small interface charge transfer from the iron to the aluminum (Table 3). The occupation of the Fe 4p states of the interface Fe is less than that of the bulk while Al 3p has more electrons than the corresponding bulk value, which indicates interactions between the Fe 4s, 4p and the Al 3s, 3p states. There are small charge oscillations for both Fe and Al parts, as shown in Table 3. The charge converges to the bulk value from the third layer. The interfacial aluminum has a negative moment ($-0.09\mu_B$), which mainly originates from the Al 3p states. The magnetic moment for the interface iron is also smaller than the bulk value. The layer-resolved occupations for the 3d states and magnetic moments for the Al–Fe multilayer system are shown in Fig. 3 and compared with the analogous Au–Fe multilayer system [11]. The behavior of the layer resolved Fe 3d occupations and the magnetic moments is very similar except for the interface iron layer.

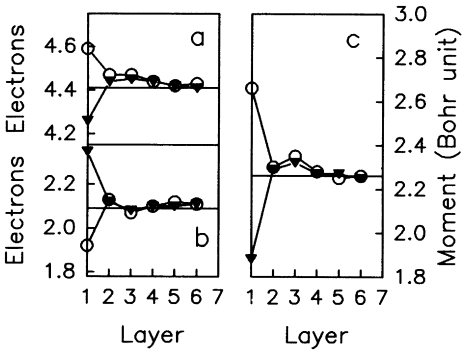

Fig. 3. Electrons in Fe 3d states for: (a) the majority direction; (b) the minority direction; and (c) the magnetic moments. The circles represent the Au–Fe multilayer system [11] and the triangles the Al–Fe (triangles) multilayer system.

Fig. 4 shows the layer-resolved densities of states for the Fe–Al multilayer. The density of states of the interface Al is very low. It is noted that Fe 3d bands of the interface Fe for both spin-directions have the widths almost the same as the bulk, which is in contrast to narrowed 3d bands for the clean Fe(001) surface or the interface Fe of the Au–Fe system.

4. Discussion

For the Fe–Al compounds the alloying of iron with aluminum causes the reduction of the magnetic moments, which is believed to be due to the charge transfer from the aluminum to the iron 3d minority orbitals [30,31]. Sundararajan et al. [32] performed calculations employing the atomic sphere approximation for the inter-metallic compound FeAl, CoAl and NiAl and concluded that there is a charge transfer (about 0.27 electrons) from aluminum to the transition metals (M) due to the different electronegativities. They attributed this to the energy level difference between atomic levels of Al and those of the transition metals, i.e. the Al 3p lies above the M 4s, while Al 3s lies above the M 3d.

The calculations for the Fe–Al multilayer system show that there is a small charge transfer from the interface Fe to the interface Al. The charge transferred (0.05 electrons per Al) is smaller than that for the Au–Fe multilayer structure (about 0.16 electrons per Au [11]), which is corresponding well to the more electronegative character of Au (2.4) compared to Al (1.5). It is noted that the charge transfer is from the interface Fe to the interface Al, while Fe is more electronegative than Al (1.8–1.5). Charge transfers cannot be uniquely defined and usually it is assumed that the positive species shrink while the negative ones expand. The charge found in, i.e. a Wigner–Seitz sphere depends on the choice of radii. In Ref. [32] equal sphere radii were employed, while in this work radii for Fe and Al used are equal to their corresponding bulk values. Compared with the bulk values, the interface Fe has less 4s and 4p electrons and a little more net 3d electrons: 4.26 electrons for majority orbitals (compared with 4.41 electrons for the bulk Fe) and 2.35 electrons for the minority orbitals (compared with the bulk value 2.09). As shown in Table 3, the interface Al has a little smaller occupation (about 0.03 electron less) for the 3s states and more for the 3p states (about 0.07 electrons more). The net result is that there is a charge transfer from the interface iron to the aluminum, as shown in Table 3.

The charge transfer is not the driving force behind the decreasing magnetic moments from a clean iron (001) surface, through a gold covered surface, the bulk iron and finally to an aluminum terminated surface. The underlying

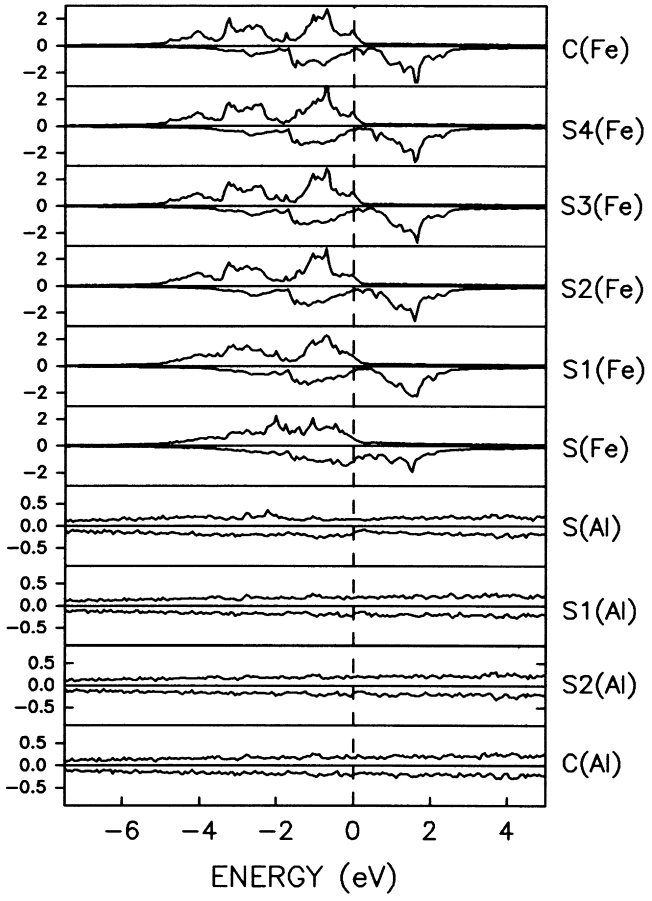

Fig. 4. Layer-resolved DOS for the Fe–Al multilayer system.

trend is the reduction of the exchange splitting of the iron 3d states through increasing hybridization. Clearly a clean iron surface has a much reduced degree of hybridization as compared with bulk iron because of its reduced coordination. This is directly reflected in the exchange splitting of the 3d states: 2.66 eV for the clean iron (001) surface, as compared with 2.15 eV for the bulk iron. Covering a clean surface with a noble metal like gold leads to a reduction of the exchange splitting of the clean surface value to 2.41 eV. A much stronger reduction is induced by the hybridization with a free electron metal like Al. Here as exchange splitting of 1.94 eV is found. The magnetic moments follow this trend in exchange splitting, of course.

Isshiki et al. found that the interface Fe layer has a strongly enhanced magnetic moment ($3.3\mu_B$) for the Fe_2/Al (001) system. They concluded that the backing effect with Al on the magnetism of the Fe film is to enhance the magnetic moment of the interface Fe. That was believed to be due to the decreasing of the population of the minority spin 3d orbital and the increasing of the electrons in the Fe 4p orbital, which comes from the mixing of the Fe 4s and 4p orbitals with the 3s and 3p orbitals of the Al substrate [22]. However, the *a*-axis of the iron layers was expanded by $\sqrt{2}$, as shown in Fig. 1 in [22]. Our calculations show that the interactions between Fe 3d and the very delocalized Al 3s, 3p states reduce the magnetic moment of the interface Fe layer. These conclusions are consistent with the calculated results for an Ni overlayer or two Ni overlayers on an Al (001) substrate [24], in which the interface Ni has reduced magnetic moment as compared with the bulk value.

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